ELSEVIER
Available online at www.sciencedirect.com
ScienceDirect
Energy Procedia 36 (2013) 401 – 407
Energy Procedia

TerraGreen 13 International Conference 2013 - Advancements in Renewable Energy and Clean Environment

Effect of Manganese concentration in the $Cd_{1-x}Mn_xTe$/CdTe Tandem structure on photovoltaic energy conversion

A. Aissat [a*], M. El Bey[a], M. Fathi[b], and J.P. Vilcot[c]

[a] LATSI Laboratory, Faculty of the Engineering Sciences, university Saad Dahlab Blida, BP270, 09.000, Algeria
[b] Semiconductor Technology Research Center for Energy, B.P.140 Alger Sept Merveilles, 16027 Algiers, Algeria
[c] Institut d'Electronique, de Microélectronique et de Nanotechnologie (IEMN), UMR CNRS 8520, Université des Sciences et Technologies de Lille 1, Avenue Poincarré, BP 60069,
59652 Villeneuve d'Ascq, France

Abstract

The photovoltaic electricity is obtained by direct conversion of sunlight into electricity by solar cells. The objective of this work is the study and simulation of a Tandem photovoltaic structure based on $Cd_{1-x}Mn_xTe$ as top material cell. This paper describes the optimization of energy efficiency for $Cd_{1-x}Mn_xTe$ thin films deposited by epitaxy on CdTe substrat. We present the impact of the manganese concentration in $Cd_{1-x}Mn_xTe$ thin films on solar cells performances. Our study includes simulation results to show the conversion efficiency and main performances factors as function of the manganese concentration.

Keywords: photovoltaic; $Cd_{1-x}Mn_xTe$; solar cells,

1. Introduction

Specific properties of CdTe made it as a perfect material for some applications, e.g solar cells, sensors, electro-optic modulators of high efficiency and photorefractive devices. This material may have both types of conductivities n and p which made diode technology [1, 2] and the field –effect transistors [3]. Semi-conductors made by CdTe as CdMnTe, have extremely exciting properties that until now not fully exploited [4]. CdTe is a ternary allow consisting of CdHgTe, which is one of the main industrials for infrared detection. CdZnTe is used as substrate for the deposition epitaxy HgCdTe layers and as a nuclear detector, which suggest a great potential application mainly for medical purposes. Physic of semi-conductors development is around the porous silicon and semi-conductors structures II-VI and III-V. Various quantum hetero-structures more or less complex (well , wires, self-organized quantum dots, laser structures , microcavities) are developed with II-VIT ellurides family (CdTe , ZnTe , MnTe , MgTe) and Nitrides with more large gap (GaN, InN,AlN). This work focuses on the main electrical and optical properties of CdMnTe alloy (with the incorporation of manganese). We will study the influence of the manganese incorporation on the characteristics of CdMnTe/CdTe structure: the band gap energy, transition energy, the strain, the reflection coefficient, the reflective index and the optical power emitted. This paper presents the structure and principle of cell photovoltaic's operation. We then give the electrical parameters of a cell-based structure of our $Cd_{1-x}Mn_xTe$/CdTe. We can identify several electronic parameters of an alloy, by linear interpolation of binary parameters parents who compose it, from the relationship of "Vegard's law":

$$P(A_{1-x-y}B_xC_yD)=(1-x-y)PAD+ xPBD+ yPCD \qquad (1)$$

1876-6102 © 2013 The Authors. Published by Elsevier Ltd. Open access under CC BY-NC-ND license.
Selection and/or peer-review under responsibility of the TerraGreen Academy
doi:10.1016/j.egypro.2013.07.046

2. **Theoretical approach**

2.1. Lattice parameter

The lattice parameter is defined as the distance between two consecutive lattices. The table 1 [5,6] gives the lattice parameters in the zinc-blend structure of our material .

Table 1. Lattice parameter of used binary materials

compound	a(A°)
CdTe	6.481
MnTe	6.337

The lattice parameter of $Cd_{1-x}Mn_x$ is calculated using Vegard's law

$$a_{Cd(1-x)Mn(x)Te}= (1-x)a_{CdTe} + x\ a_{MnTe} \quad (2)$$

2 .2strains and relaxation

When the epitaxial growth of a material on a substrate of different lattice parameter, a compressive or a biaxial expansion strain occurs on the layer epitaxed, which is accompanied by an elastic energy accumulation. Beyond a critical thickness, the elastic energy stored is sufficient to generate structural defects which partially relax the strain in the crystal. The material then tends to resume its lattice parameter, and dislocations appear at the interface (plastic relaxation).The critical thickness depends directly on the difference of lattice parameter between substrate and layer [7]. Elastic deformation of network appears perpendicularly to the plan of growth (figure 1).

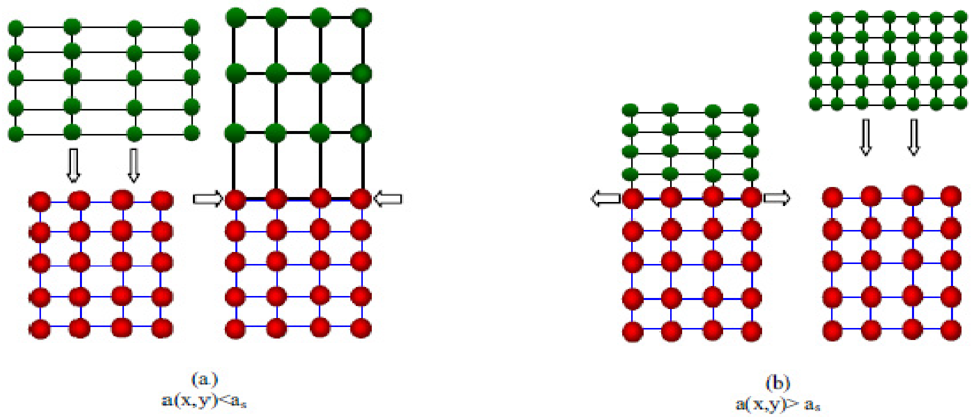

Figure 1.epitaxy of mismatch lattice parameter layer
(a) in compression and (b) in strain on a substrate that lattice parameter is a_0. [8,9]

In the case of a standard rigid substrate very thick, the constraints are substantially borne by the growing layer. Its strain rate is a function of the lattice mismatch with the substrate. This disagreement is defined by [8].

$$\epsilon = \frac{\Delta a}{a} = \frac{a_{s-a_e}}{a_s} \quad (3)$$

Where a_s and a_e are respectively the lattice parameters of substrate and the natural layer epitaxed**.** If ϵ is positive, the layer is in "tension" and if it is negative the layer is in "compression". The alloy $Cd_{1-x}Mn_xTe$ has a direct gap which varies almost linearly with Mn's composition [10]. The biaxial strain can be decomposed into a hydrostatic term and a shear component. The first changes the band gap, whereas the shears liftthe degeneracy of the valence band between heavy and light holes [7]. When the solar irradiation enters a semiconductor, a part of this radiation is reflected, another is absorbed and the last passes through the layer of material without being absorbed. The optical properties of a solid are in dependence of the conventional band diagram in reciprocal space k [11].The electric structure of CdTe shows a direct gap semiconductor, whose band structure allows important vertical radiatives transitions between valence band and conduction band. This property is the main purpose of his application in optoelectronic's field. CdTe has a wide band gap of about 1,51 eV at room temperature (300 °K), which gives a threshold optical absorption in infrared field, particurly infrared sensing and as a substrate for epitaxy of CdMnTe layers. During the path of light in the solar cell active layer, a photon can be absorbed by this layer to produce an electron-hole pair [12]. The absorption coefficient α for photon energy greater than the gap energy is given by the following formula**:**

$$\alpha = \alpha_0 \frac{\sqrt{E-E_g}}{E} \tag{4}$$

where $\alpha_0 = 5.10^5 cm^{-1}$

The variation of refractive index is calculated using empirical Herve and Vandamme's formula, which is a function of band gap energy:

$$n = \sqrt{1+\left(\frac{A}{E_g+B}\right)^2} \tag{5}$$

where A and B having the values 6.13 and 3.4eV, respectively. In fact, the semiconductor refractive index is fundamental physical parameters which characterize optical and electrical property [13].

2.2.1 Reflection

The reflection law says that for specular reflection, the angle at which the wave is incident on surface equals the angle at which it is reflected. The reflection coefficient is defined by the following formula:

$$R = \left(\frac{1-n}{1+n}\right)^2 \tag{6}$$

Where n is the layer reflective index.

3. Solar cell parameters :

The solar cell is just another photodiode that operates without external bias and supply its photocurrent in a load. Definition of cell's parameters is performed from the current voltage characteristic. We can observe that, in darkness, the solar cell has diode behavior. Under illumination, the various parameters characterizing the photovoltaic cell can be determined in according to the shape of the curve in the fourth quadrant:
There is [14]:

$$I = I_{ph} - I_S\,(e^{eV/KT} - 1) \tag{7}$$

The first term of the expression is the photo-current; the second is a direct current resulting from the bias of the diode in the forward sense by the voltage V which appears across the load resistor. The photocurrent is a function of the absorption coefficient, the incident flow and the width of the depletion region. To calculate photocurrent we plot the variation of the number of photons absorbed with respect of Manganese concentration.

3.1 Short-circuit current $I_{CC.}$

This is the current supplied by the cell when the voltage across its terminal is zero. It increases with the intensity of illumination of the cell and depends on the illuminated surface, the radiation wavelength, the carrier mobility and temperature [15]. The short circuit current is the obtained current when the cell terminals are short circuited (V= 0).It decreases with the manganese concentration**.**

3.2 Open circuit voltage , V_{oc}

The open circuit voltage represents the voltage across the cell under illumination without charging circuit. It depends on the type of solar cell (pn junction, Schottky junction), materials of active layer and nature of contacts. It also depends on the cell illumination. That is the maximum potential that the cell can provide when the current is zero. It is given by :

$$V_{OC} = \frac{E_g}{q} - \frac{KT}{q} ln(\frac{I_0}{I_{cc}}) \quad (8)$$

3.3 Power output :

The power supplied by the battery is given by the product V I.

$$P= VI = V (I_{ph}-I_S(e^{eV/KT}- 1)) \quad (9)$$

This power is maximum at the point P_m , defined by dp/dv = 0 ,

i.e $$I_{ph}- I_S(e^{eV/KT}-1) - I_S\frac{eV}{KT} e^{\frac{eV}{KT}} = 0 \quad (10)$$

The voltage V_m and I_m at the point P_m are given by

$$\left(1 + \frac{eV}{KT}\right) e^{\frac{eV_m}{KT}} = 1 + \frac{I_{ph}}{I_S} \quad (11)$$

$$I_m= I_S \frac{eV_m}{KT} e^{\frac{eV_m}{KT}} \quad (12)$$

The power output is then given by the product V_mI_m as

$$P_m = V_mI_m = FF\ V_{oc}I_{cc} \quad (13)$$

FF is the form factor.

3.4 Form factor

The parameter FF is the fill factor or form factor; it measures the rectangular character of the curve I-V. This is a ratio that reflects the quality of its I(V) curve form. It is defined by the following equation [12].

$$FF = \frac{V_mI_m}{V_{oc}I_{cc}} \quad (14)$$

3.5 Efficiency

The conversion efficiency for solar cells refers to the ability of the cell to cover the photon energy [16]. The efficiency of the solar cell is given by the ratio of the maximum power available to the incident radiation power. It represents the external energetic efficiency of power conversion.

$$\eta = \frac{P_m}{P_0} = FF \frac{V_{oc}I_{cc}}{P_0} \quad (15)$$

The expression shows that the solar cell performance is resulting directly from the three parameters values I_{cc},V_{oc} and FF. The parameters are from part a function of the specific properties of the material, such that gap, absorption and reflection coefficients, diffusion length of the carrier or surface recombination velocity; and from other part technological parameters such the depth of junction, width of the space charge zone and the presence of parasitic resistances.

4. Results and discussion

The figure 2represents the variation of the lattice mismatch as a function of the x% Manganese concentration. We see a small mismatch between the epitaxial layer $Cd_{1-x}Mn_xTe$ and CdTe substrate. For x=0% we have a lattice mismatch ϵ=0 and for x=100% then ϵ=2.2 % also the incorporation of Manganese Mn causes a tensile strain. The figure 3 shows the variation of the strained structure’s energy gap depending on the manganese concentration x. The layer is subjected to a tensile strain, so the heavy holes‘s band is below the light holes’ band and the absorption can be for only incident photon energy greater than 1.6eV. The figure 4 represents change of absorption coefficient as a function of energy incident light for different values of manganese concentration. The increase in the concentration of Mn leads a reduction absorption coefficient. For a photon energy E_{ph}=3eV, x=20% the absorption is $\alpha=1.7210^5 cm^{-1}$ and for x=50 % it is $\alpha_2=1.2710^5 cm^{-1}$.We shows that the absorption decreases as $\Delta\alpha=0.4510^5 cm^{-1}$. We also note that for x=20% the maximum absorption is $\alpha_{max}=1.8810^5 cm^{-1}$ and for x=50%, $\alpha_{max}=1.4610^5 cm_{-1}$; we have then a decrease of $\Delta\alpha_{max}=0.4210^5 cm^{-1}$.The figure 5 illustrates the variation of the refractive index as a function of manganese concentration. The refractive index of the material does not exceed value of n=2.9, so we can say that the reflectivity decreases with manganese concentration rising. The figure 6 shows current- voltage characteristic for several concentrations of Mn. The increasing of manganese concentration leads to a reduction of the short circuit. For x=10 %, J_{cc}=65.41 mA/cm^2 and for x=70 %, J_{cc}=49.95mA/cm^2; we have then a decreasing of ΔJ_{cc}=15.96mA/cm^2.The figure 7shows the variation of the power delivered by the cell as the function of bias voltage for different manganese percentages. We notice a decrease in power in accordance with the increase of x. For an 25% manganese increasing in structure, we find that there‘s a significant reduction of the maximum power ΔP =5.2mw/cm^2.We see a reduction in cell efficiency by increasing the percentage of manganese in the active layer. For x =0% the efficiency is 20.25% and for x=10% it is 14.01. We need to find a compromise between the manganese concentration and strain to achieve a reliable structure.

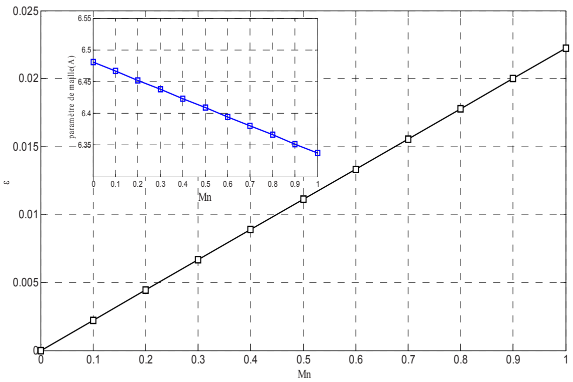

Figure 2. change mismatch versus manganese concentration in the $Cd_{1-x}Mn_xTe$ / CdTe structure.

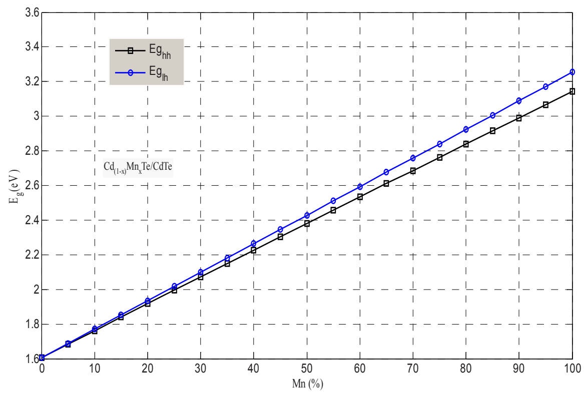

Figure 3 . band gap energy variation of the strained structure as function of manganese concentration.

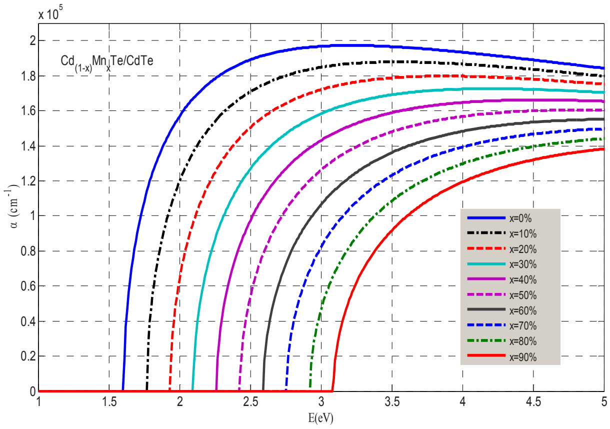

Figure 4 .variation of absorption as function of photon energy.

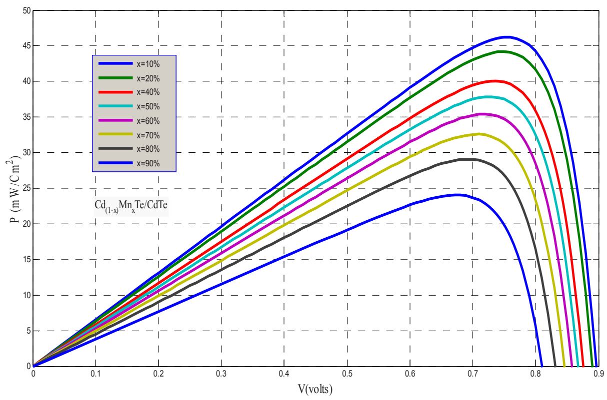

Figure 5. current-voltage characteristic of CdMnTe structure

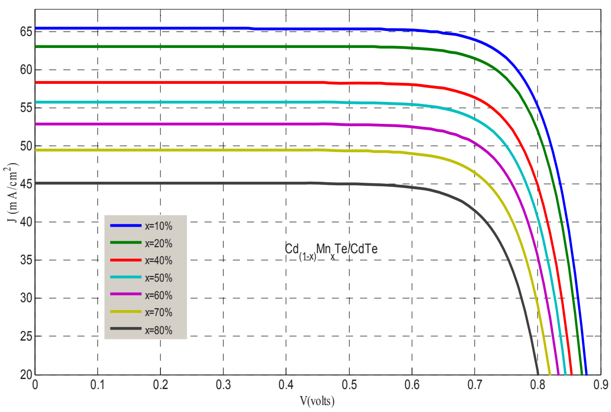

Figure 6 . power delivered by cell based on CdMnTe.

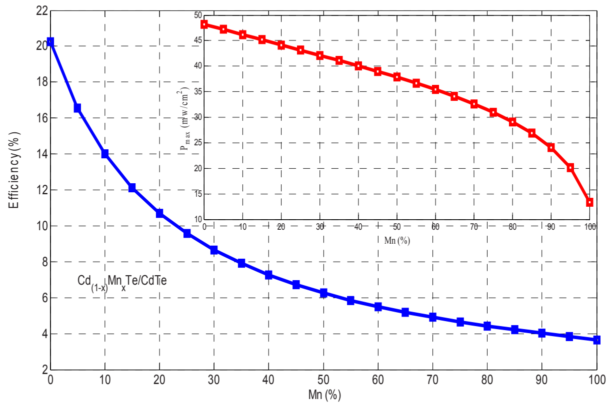

Figure 7.conversion efficiency of the cell based on CdMnTe.

5. Conclusion

This work focuses on the study and simulation of electrical characteristics of a solar cell based materials ternary $Cd_{1-x}Mn_xTe$ on a substrate CdTe; either the effect of different physical and optical parameters of the cell has been explored. We considered the impact of manganese concentration on the physical parameters of the ternary and the strain effect between the two layers of $Cd_{1-x}Mn_xTe$ and CdTe. The results show that the epitaxed alloy is under low tension strain. The increasing of manganese concentration increases the gap. For optoelectronic characteristics, the incorporation of manganese reduces the absorption coefficient. We determine the influence of Mn on the I(V) characteristic and the power delivered by the cell. The obtained results allow the calculation of maximum efficiency of the cell which reaches 20 %.

References

[1] N. Abbas Shaha, A. Alia, A.K.S. Aqilib, A. Maqsooda, Physical properties of Ag-doped cadmium telluride thin films fabricated by closed-space sublimation technique, Journal of Crystal Growth 290 452–458 (2006)
[2] Nazar Abbas Shah, Abid Ali, AsghariMaqsood, Preparation and Characterization of CdTe for Solar Cells, Detectors, and Related Thin-Film Materials, ournal of Electronic Materials Volume 37, Issue 2, pp 145-151 (2008)
[3] Y.M. Kim, M. Yoon, I.-W. Park, Y.J. Park, Jong H. Lyou, Synthesis and magnetic properties of Zn12xMnxO films prepared by the sol–gel method, Solid State Communications 129 175–178 (2004)
[4]M.G. Simeone, S. Viticoli, Crystal growth and characterization of $Mn_xCd_{1-x}Ga_2Se_4$: A new family of diluted magnetic semiconductors, Volume 23, Issue 8, 1219–1225 (1988)
[5] Philippe BARATE: "Generation and optical detection of spin waves in CdMnTe quantum wells n doped", Montpellier II University, France (2010).
[6] Landolt-Börstein: `Numerical data and functional relationships in science and Technology', Springer-Verlag Berlin, (1982)
[7] Alexandre ARNOULT : `Dopage par modulation d'hétérostructures de semiconducteurs II-VI semimagnétiques en épitaxie par jets moléculaires', Université Joseph Fourier, (1998).
[8] Damien BORDEL:"Development of new compliant substrates for the hetero-epitaxy of semiconductors", ECOLE CENTRALE DE LYON, France (2007).
[9] A. Aissat, S. Nacer and H. Aliane, J.P. Vilcot "Long Wavelength Determination of a strained Quantum Well Structure Based on GaxIn1-x-yAsySb1-y /GaSb for gas detection" 978-1-4577-0069-9/11/$26.00 © IEEE (2011)
[10] David Plantier: "Raman spectroscopic study of low-energy excitations in semiconductors subjected to intense magnetic fields", Joseph Fourier University, France (2003).
[11] H. Koezuka, A. Tsumura, T. Ando , Field-effec transistor with polythiophene thin film, Synthetic Metals, Volume 18, Issues 1–3, 699–704 (1987)
[12] loïcbailly"Flexible organic photovoltaic cells having large surface", Bordeaux I University, France (2010).
[13] S. Mnasri, S. Abdi-Ben Nasrallah, N. Sfina, N. Bouarissa et M. Said : `Electronic, lattice vibration and mechanical properties of CdTe, ZnTe, MnTe, MgTe, HgTe and their ternary alloys', Monastir, Tunisia, (2009)
[14]José Miguel Navarro : "Transparent Organic Photovoltaic Cells In The Visible", (2008).
[15] F.T. Reis , D. Mencaraglia, S. OouldSaad, I. Séguy, M. Oukachmih, P. Jolinat, P. Destruel, Characterization of ITO/CuPc/AI and ITO/ZnPc/Al structures using optical and capacitance spectroscopy, Synthetic MetalsVolume 138, Issues 1–2, 2, 33–37 (2003)
[17] PETIBON Stéphane :"New distributed architectures management and energy conversion for photovoltaic applications", Toulouse University, France (2009).